Explicit Newmark algorithm for rotational dynamics

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Abstract

The explicit Newmark algorithm for vector-space dynamics is the workhorse of structural dynamics. This paper derives the counterpart of the explicit vector-space algorithm for the rotational dynamics of rigid bodies from the midpoint rule in the Lie incarnation. By introducing discrete, concentrated impulses we can approximate the forcing imparted to the system over the time step, and thus we formulate two adjoint explicit first-order integrators. These may be composed to yield a second-order integrator which inherits the symplecticity and momentum conservation of the first-order integrators. In this manner, we get the classical Newmark algorithm for translational motion (vector space dynamics), or the rotation-group Newmark for rigid body rotation problems.

Keywords: Rigid body dynamics; Explicit time integration; Midpoint algorithm; Symplectic Euler; Newmark; Midpoint Lie

1. Introduction

For some time now many researchers have tried to come up with an explicit Newmark for the 3-D rotations of rigid bodies. The resulting algorithms were honored with the Newmark name, but so far none could claim the excellent variational structure of the vector-space Newmark.

The vector-space Newmark algorithm may be written as a composition of two first-order algorithms, the symplectic Euler and its adjoint [1]. As we shall show, this composition may be interpreted in terms of an approximation of the midpoint rule: the implicit form of the midpoint impulse may be approximately replaced by concentrated impulses at known configurations, which leads to explicit algorithms as approximate midpoint rules. We point out that this mechanically inspired derivation yields the well-known second-order explicit Newmark algorithm in the vector space setting, but, as we show here, when the midpoint rule is interpreted in the Lie sense on the rotation group *SO* (2), also a remarkably accurate integrator for rigid body rotations. This rotation-group integrator is the *direct counterpart* of the explicit Newmark algorithm in the vector-space setting, and comes with corresponding properties of symplecticity and angular momentum conservation.

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Computational Fluid and Solid Mechanics 2005
K.J. Bathe (Editor)

2. Vector-space dynamics

The initial value problem for a mechanical system (for instance a system of interacting particles) described by a vector of configuration variables (displacements) $\mathbf{u} \in \mathbb{R}^n$ may be put as

$$\begin{aligned} \dot{\mathbf{p}} &= \mathbf{f}, \quad \mathbf{p}(0) = \mathbf{p}_0 \\ \dot{\mathbf{u}} &= \mathbf{M}^{-1}\mathbf{p}, \quad \mathbf{u}(0) = \mathbf{u}_0 \end{aligned} \tag{1}$$

where $\dot{\mathbf{p}}$ is the rate of linear momentum, $\dot{\mathbf{u}}$ is the velocity, and $\mathbf{f} = \mathbf{f}(\mathbf{u}, t)$ is the applied force. We shall assume a time-independent mass matrix $\mathbf{M}$. The initial values are $\mathbf{p}_0$, and $\mathbf{u}_0$.

The midpoint approximation to Eq. (1) is written as

$$\begin{aligned} \frac{\mathbf{p}(t+\Delta t) - \mathbf{p}(t)}{\Delta t} &= \mathbf{f}(\mathbf{u}(t+\Delta t/2), t+\Delta t/2) \\ \frac{\mathbf{u}(t+\Delta t) - \mathbf{u}(t)}{\Delta t} &= \mathbf{M}^{-1}\left(\frac{\mathbf{p}(t+\Delta t) + \mathbf{p}(t)}{2}\right) \end{aligned}$$

The first equation of Eq. (1) may be recognized as a one-point quadrature applied to the impulse integral

$$\mathbf{p}(t+\Delta t) \quad = \quad \mathbf{p}(t) + \int_t^{t+\Delta t} \mathbf{f}(\mathbf{u}(\tau), \tau) d\tau$$

$$\approx \quad \mathbf{p}(t) + \Delta t \mathbf{f}\left(\frac{\mathbf{u}(t+\Delta t)+\mathbf{u}(t)}{2}, t+\frac{\Delta t}{2}\right) \tag{2}$$

This result allows us to write

$$\frac{\mathbf{u}(t+\Delta t)-\mathbf{u}(t)}{\Delta t} = \mathbf{M}^{-1}\left[\mathbf{p}(t) + \frac{\Delta t}{2}\mathbf{f}\left(\frac{\mathbf{u}(t+\Delta t)+\mathbf{u}(t)}{2}, t+\frac{\Delta t}{2}\right)\right] \tag{3}$$

with a clear mechanical interpretation: the term in the brackets on the right is an approximation of the midpoint momentum,

$$\begin{aligned} \mathbf{p}(t+\Delta t/2) &= \mathbf{p}(t) + \int_t^{t+\Delta t/2} \mathbf{f}(\mathbf{u}(\tau),\tau)d\tau \\ &\approx \mathbf{p}(t) + \tfrac{\Delta t}{2}\mathbf{f}\left(\frac{\mathbf{u}(t+\Delta t)+\mathbf{u}(t)}{2}, t+\frac{\Delta t}{2}\right) \end{aligned} \tag{4}$$

This may be explained in mechanical terms by recourse to the concept of discrete impulses that replace the integral of the continuous forcing. In particular, Eqs. (2) and (3) may be understood as exact evaluations of the momentum with discrete impulses $\frac{\Delta t}{2}\mathbf{f}\left(\frac{\mathbf{u}(t+\Delta t)+\mathbf{u}(t)}{2}, t+\Delta t/2\right)$ imparted to the system at times $(t + \Delta t/2)_-$ and $(t + \Delta t/2)_+$. (Interpret τ_- and τ_+ as immediately to the left of τ or immediately to the right of τ.)

Clearly, the above midpoint algorithm is implicit, since the forcing needs to be evaluated at the unknown geodesic midpoint $\frac{\mathbf{u}(t+\Delta t)+\mathbf{u}(t)}{2}$. To unravel this implicitness, we may consider a different distribution of the discrete impulses in time. In particular, the total impulse may be delivered at the end of the time step, that is at $(t + \Delta t)_-$, in which case

$$\int_t^{t+\Delta t/2} \mathbf{f}(\mathbf{u}(\tau),\tau)d\tau \approx 0$$

On the other hand, the impulse may be imposed at the start of the time step, that is at $(t + \Delta t)_+$, and

$$\int_t^{t+\Delta t/2} \mathbf{f}(\mathbf{u}(\tau),\tau)d\tau \approx \Delta t \mathbf{f}(\mathbf{u}(t),t)$$

In this manner, we obtain two *explicit* algorithms. The first one, $\mathbf{\Phi}_{\Delta t}$, may be recognized as the symplectic Euler method, and the second, $\mathbf{\Phi}^*_{\mathrm{h}}$, as its adjoint.

$$\mathbf{\Phi}_h\begin{pmatrix}\mathbf{p}_t\\ \mathbf{u}_t\end{pmatrix} = \begin{pmatrix}\mathbf{p}_{t+h}\\ \mathbf{u}_{t+h}\end{pmatrix} = \begin{pmatrix}\mathbf{p}_t + h\mathbf{f}_t\\ \mathbf{u}_t + h\mathbf{M}^{-1}\mathbf{p}_{t+h}\end{pmatrix}$$

$$\mathbf{\Phi}^*_h\begin{pmatrix}\mathbf{p}_t\\ \mathbf{u}_t\end{pmatrix} = \begin{pmatrix}\mathbf{p}_{t+h}\\ \mathbf{u}_{t+h}\end{pmatrix} = \begin{pmatrix}\mathbf{p}_t + h\mathbf{f}_{t+h}\\ \mathbf{u}_t + h\mathbf{M}^{-1}\mathbf{p}_t\end{pmatrix}$$

where we use subscripts instead of arguments in parentheses. These algorithms are *symplectic* [1], and, in the absence of external forcing, *momentum conserving*. Their accuracy is only linear in the time step, but their composition preserves both symplecticity and momentum conservation, and yields a second-order accurate algorithm [1]

$$\mathbf{\Xi}_{\Delta t} = \mathbf{\Phi}^*_{\Delta t/2} \circ \mathbf{\Phi}_{\Delta t/2} \tag{5}$$

This algorithm may be recognized as the well-known explicit Newmark ($\gamma = 1/2$ and $\beta = 0$).

3. Dynamics on the rotation group

The equation of motion of a rigid body rotating about a fixed point is written in the spatial frame as $\dot{\pi} = \mathbf{RT}$, where $\pi = \mathbf{R\Pi}$ is the spatial angular momentum. Integrating the spatial equation of motion, and converting back to the body frame, we may write the equation of motion in the body frame in integral form as

$$\mathbf{\Pi}(t) = \exp[-\mathrm{skew}[\mathbf{\Psi}]]\left(\mathbf{\Pi}(t_0) + \mathbf{R}^T(t_0)\int_{t_0}^{t}\mathbf{R}(\tau)\mathbf{T}(\tau)d\tau\right) \tag{6}$$

where $\exp[-\mathrm{skew}[\mathbf{\Psi}]] = \mathbf{R}^T(t)\mathbf{R}(t_0)$ is the incremental rotation through vector $-\mathbf{\Psi}$. Differentiating (6), and by comparison with the original differential equation of motion, we obtain

$$\dot{\mathbf{\Psi}} = \left(d\exp_{-\mathrm{skew}[\mathbf{\Psi}]}\right)^{-1}\mathbf{I}^{-1}\mathbf{\Pi}$$

where $d\exp_{-\mathrm{skew}[\mathbf{\Psi}]}$ is the differential of the exponential map [2]. The initial value problem may be therefore rewritten as

$$\dot{\mathbf{\Pi}} = -\mathrm{skew}[\mathbf{I}^{-1}\mathbf{\Pi}]\mathbf{\Pi} + \mathbf{T}, \quad \mathbf{\Pi}(0) = \mathbf{\Pi}_0$$

$$\dot{\mathbf{\Psi}} = \left(d\exp_{-\mathrm{skew}[\mathbf{\Psi}]}\right)^{-1}\mathbf{I}^{-1}\mathbf{\Pi}, \quad \mathbf{\Psi}(0) = \mathbf{0}$$

In analogy to Eq. (3) we may write the midpoint approximation to the second equation of the above initial value problem as ($\mathbf{\Psi}_t = \mathbf{0}$)

$$\frac{\mathbf{\Psi}_{t+\Delta t}}{\Delta t} = \left(d\exp_{-\mathrm{skew}[\frac{1}{2}\mathbf{\Psi}_{t+\Delta t}]}\right)^{-1}\mathbf{I}^{-1}\mathbf{\Pi}_{t+\Delta t/2}$$

which may be simplified by noting

$$d\exp_{-\mathrm{skew}[\frac{1}{2}\boldsymbol{\Psi}_{t+\Delta t}]}\boldsymbol{\Psi}_{t+\Delta t}=\boldsymbol{\Psi}_{t+\Delta t}$$

to give

$$\frac{\boldsymbol{\Psi}_{t+\Delta t}}{\Delta t}=\mathbf{I}^{-1}\boldsymbol{\Pi}_{t+\Delta t/2}$$

This equation needs to be solved for the rotation vector, and, along the lines of the argument that follows Eq. (4), the midpoint approximation of the angular impulse

$$\boldsymbol{\Pi}_{t+\Delta t/2}=\boldsymbol{\Pi}_t+\frac{\Delta t}{2}\exp\left[\tfrac{1}{2}\mathrm{skew}[\boldsymbol{\Psi}_{t+\Delta t}]\right]\mathbf{T}_{t+\Delta t/2}$$

would result in an implicit algorithm (algorithm **LIE-MID[I]** referred to in the Examples section). Using discrete impulses applied at the start or at the end of the time step, we get two explicit algorithms, depending on the chosen approximation of the impulse. For the impulse applied at the start of the time step we obtain the counterpart of the symplectic Euler integrator $\boldsymbol{\Phi}_h$

$$\tilde{\boldsymbol{\Phi}}_h\begin{pmatrix}\boldsymbol{\Pi}_t\\ \mathbf{R}_t\end{pmatrix}=\begin{pmatrix}\boldsymbol{\Pi}_{t+h}\\ \mathbf{R}_{t+h}\end{pmatrix}=\begin{pmatrix}\exp[-\mathrm{skew}(\boldsymbol{\Psi}_{t+h})](\boldsymbol{\Pi}_t+h\mathbf{T}_t)\\ \mathbf{R}_t\exp[\mathrm{skew}(\boldsymbol{\Psi}_{t+h})]\end{pmatrix}$$

where $\boldsymbol{\Psi}_{\mathrm{t+h}}$ solves

$$\tfrac{1}{h}\mathbf{I}\boldsymbol{\Psi}_{t+h}=\exp\left[-\mathrm{skew}(\tfrac{1}{2}\boldsymbol{\Psi}_{t+h})\right]\ (\boldsymbol{\Pi}_t+h\mathbf{T}_t)$$

On the other hand, the total torque impulse applied at the end of the time step yields the adjoint method

$$\tilde{\boldsymbol{\Phi}}^*_h\begin{pmatrix}\boldsymbol{\Pi}_t\\ \mathbf{R}_t\end{pmatrix}=\begin{pmatrix}\boldsymbol{\Pi}_{t+h}\\ \mathbf{R}_{t+h}\end{pmatrix}=\begin{pmatrix}\exp[-\mathrm{skew}(\boldsymbol{\Psi}_{t+h})](\boldsymbol{\Pi}_t+h\mathbf{T}_{t+h})\\ \mathbf{R}_t\exp[\mathrm{skew}(\boldsymbol{\Psi}_{t+h})]\end{pmatrix}$$

where $\boldsymbol{\Psi}\mathrm{i}_{\mathrm{t+h}}$ solves

$$\tfrac{1}{h}\mathbf{I}\boldsymbol{\Psi}_{t+h}=\exp\left[-\mathrm{skew}(\tfrac{1}{2}\boldsymbol{\Psi}_{t+h})\right]\ \{\boldsymbol{\Pi}_{\mathrm{t}}$$

Both algorithms are first-order, symplectic, and momentum conserving in the absence of external torques. Even though an *implicit* equation needs to be solved in order to solve for the incremental rotation vector (the implicit character is due to the configuration variables belonging to $SO(3)$, a manifold, not to a vector space as for the algorithms $\boldsymbol{\Phi}_h$ and $\boldsymbol{\Phi}_{h^*}$, the algorithms are *explicit* in the torque evaluations, which was our goal all along.

As before, the composition of these two algorithms in one time step provides us with a second-order accurate algorithm, which is an analogy of the explicit Newmark algorithm for the vector space dynamics

$$\tilde{\boldsymbol{\Xi}}_{\Delta t}=\tilde{\boldsymbol{\Phi}}^*_{\Delta t/2}\circ\tilde{\boldsymbol{\Phi}}_{\Delta t/2}$$

We shall call the above first-order algorithms the explicit midpoint Lie variant 2 ($\tilde{\boldsymbol{\Phi}}_h$) and 1 ($\tilde{\boldsymbol{\Phi}}^*_{\mathrm{h}}$) respectively. These algorithms are not simply the symplectic Euler and its adjoint. They all reduce to the full midpoint Lie algorithm for torque-free motion. Application of the discrete impulses at points different from the midpoint distinguish them from the implicit midpoint Lie rule. Consequently, the explicit Newmark algorithm could also be called the alternating midpoint Lie algorithm ($\tilde{\boldsymbol{\Xi}}_{\Delta t}$).

4. Example

As an illustration, we consider the *slow* symmetrical top with total mass in a uniform gravitational field. Fig. 1 illustrates the remarkable accuracy of the present explicit midpoint Lie (explicit Newmark) algorithm, $\tilde{\boldsymbol{\Xi}}_{\Delta t}$, in comparison with selected state-of-the-art high-performance algorithms. The tip of the vector pointing along the axis of the slow top from the attachment point is projected onto the plane perpendicular to the direction of gravity. The reference solution is shown in dotted line. The numerical solutions are obtained with $\Delta t = 0.1$, which corresponds to incremental rotations within the time step of about 30°. Our algorithm $\tilde{\Xi}_{\Delta t}$ captures the overall character of the trajectories extremely well, much better in fact than the canonical implicit algorithms. The other explicit algorithm used for comparison, **SW**, loses stability early on (the **SW** algorithm is neither energy nor symplectic form conserving).

5. Conclusions

We have presented an approach to the construction of mechanical integrators for general 3-D rotations that are explicit in the evaluation of the forcing. The starting point is the midpoint (implicit) rule and the integral of the forcing is approximated with concentrated impulses. The resulting algorithms conserve momentum, are symplectic, first-order, and they are adjoint. Consequently, their composition leads to a second-order algorithm, which may be readily interpreted as the rotation-group explicit Newmark integrator. This is the true heir of the vector-space Newmark, with the desired variational structure and excellent performance. Numerical evidence suggests that it is the best explicit second-order integrator to date, which is in line with what is known about the vector-space version.

Acknowledgment

Support for this research by a Hughes–Christensen award is gratefully acknowledged.

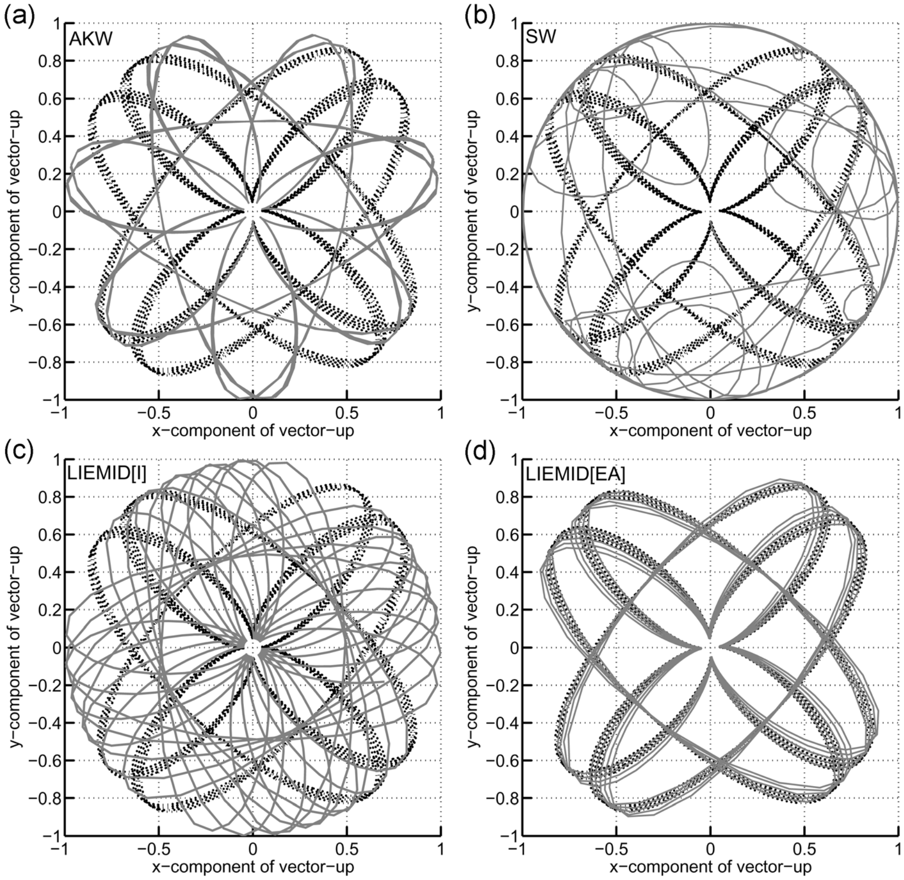

Fig. 1. Slow Lagrangian top: components of the unit vector along the axis of the top in the plane perpendicular to the direction of gravity. (a) **AKW**: implicit mid-point rule of Austin et al. [3]; (b) **SW**: Simo and Wong [4]; (c) **LIEMID [I]**: implicit midpoint Lie; (d) **LIEMID [EA]**: alternating explicit midpoint Lie (explicit Newmark) algorithm, $\tilde{\Xi}_{\Delta t}$.

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